8295-EN-01
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MODELLING OF AEROSOL DISPERSION BY ATMOSPHERE TURBULENCE

Belov N.N.

AEROSOL TECHNOLOGY LTD

CONTRACT NUMBER 68171 - 97 - M - 5712

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December 97 - February 98

The Research reported in this document has been made possible through the support and sponsorship of the U.S. Government through its European Research Office of the U.S. Army. This report is intended only for the internal management use of the Contractor and U.S. Government.

REPORT DOCUMENT PAGE	Form Approved OMB No. 0704-0188

I. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	25 Feb 98	Interim report, 01 December 97 - 28 February 98

4. TITLE AND SUBTITLE	5. FUNDING NUMBERS
Method of probe clouds for modelling of the aerosol dispersion in turbulence atmosphere for complicated landscape.	C - Accession No. 68171 - 97 - M - 5712

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10.SPONSORING/MONITORING AGENCY REPORT NUMBER
I I. SUPPLEMENTTARY NOTES	

12a. DISTRIBUTION/AVAILABILITY STATEMENT	12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 75 words)

Synthetic models of aerosol dispersion in atmosphere are based upon the lib streams and the method of modelling aerosol dispersion along the streamlin model is based on the method of probe clouds that come from the nozzle of generator and move along the streamline. Final differences scheme for 3D Stokes equations was improved to build the library. This method is effe modelling aerosol transport by complex air flows.

Second quarter finished with new modification of 3D computation codes - probe clouds model for non homogeneity aerosol plume.

Main results are of research group:

Preparing of new modification of synthetical modelling of aerosol dispersion ion atmosphere.

14. SUBJECT ITEMS	15. NUMBER OF PAGES
Modelling; Atmosphere; Method of probe clouds; Finite-differences scheme; probe clouds; turbulence; stream-lines	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CIASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified, For Public use	Unclassified, For Public use	Unclassified, For Public use	Non limited, For Public use

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Preacribed by ANSI Std.Z39-18
289-102

ATTACHMENT 1

CONTRACT No 68171 - 97 - M - 5712

Section II - Interim Report

Method of probe clouds for modeling of the aerosol dispersion in turbulence atmosphere on complicated landscape

This interim report devoted to preparing the effective methods of prediction of aerosol transport, which modifies concentration field. This method takes into account local convection flows and whirlwinds near obstacles. Movement of the aerosol plume near source depends from different air streams. So the most important part of modelling is description of aerosol streams and their route from the source.

Present investigation devoted to the new method for fast and accurate direct solving of 3D aerodynamics problem with complex boundary conditions. The synthetical modelling of aerosol dispersion in atmosphere is based upon the library of streams. Library contains three dimensional description of air flows. The library of flows must be big enough to contain flows around various kinds of obstacles with high precision. Each flow is modelled using final-differences scheme for three dimensional Navier-Stokes equations (without temperature). Final-differences scheme precision could be improved by dividing dynamics equations by value of average density and introducing the kinematic viscosity of air. The last replaces theoretical artificial viscosity so it is not needed. Preparation of library takes a lot of time. But when library is ready computational time needed for synthetic model is small enough to let use of this model during outdoor experimental studies.

New models of turbulence diffusion are established.

One model uses the streamline which passes through place of aerosol generator as a center line of Gaussian model of aerosol plume dispersion. This modification of Gaussian model is used for evaluation of the aerosol dispersion in atmosphere with complicated orography. Gaussian models provides quasi - homogeneous aerosol distribution inside aerosol plume. This model is good when the threshold is negligible. But it can not be used when non linear effects are investigated.

Model of another type is based on the method of probe clouds. Method of probe clouds is similar to method of markers in gasdynamics. All probe clouds come from nozzle of aerosol generator and move along the streamline. Every cloud have it's own parameters for the defined set of physical characteristics. The last is loaded from the air flows library for each moment. In this method aerosol plume is replaced with set of probe clouds. During simulation, the movement of each cloud is divided into several steps. On each step the corresponding parameters are changed to model elementary physical process. For example, the stochastic generation of clouds, transformation by turbulence diffusion and convectional transfer at small time step can be investigated. The global field of any physical parameter can be found from description of probe clouds displacement and their characteristics. The total number of clouds can be chosen to reach given precision or to compute no longer the given time period. This method is effective in modelling aerosol transport in case of wheelwinds, convection, etc. This investigation enables evaluation of complicated problem of aerosol transport during field experiment in quasi-real time. This second model is good for computation of evolution of aerosol with given precision. It is very important for aerosol optics, investigation of other non linear effects in real atmosphere.

Future plans

Receiving of the money from ERO. This is most important problem of my contracts. Up to now (6 months of preparing of the two ERO contracts) I have not any payment from ERO! I tired from pressing of Russian crimes and KGB, I can not pay to my co-workers, I can not prepare new devices, etc. I need in information help about sender of money (name, phone, fax) copy of payment documents. If this month I will unable to receive ERO money I will sale my car for supporting of this investigations. If you will can not send me money I will find another money source. In that case best partner for ERO is KGB - it will have not any problems with receiving of ERO money by cheque...
Please note that after receiving of ERO contracts:
- I lost my salary in Karpov Institute,
- I spent money of my family for supporting of investigations by ERO contracts
This month is critical for me and my colleagues. If ERO can not search safety way for payment in Russia for independent scientists - all ERO money sent to Russia will be received by Russian crimes and KGB.
Please make your schools!
Another problem - I have not clauses on software rights and clauses about disputes.
Seems ERO did not want to provide me informational support. I have KGB pressing in Russia and ERO financial and informational waving from another side.

May be ERO supports of KGB in its hunting of Russian scientists?

(3) A statement of significant administrative actions during the period reported such as personnel changes, important conferences and the like.

Belov N.N. as PI of the contract received several applications form for involving in this project from Professors and Dr. of Moscow State University. So our list of participants (only their names) of this proposal will be change without changing of money distribution between participance.

(4) Any other information considered important by the Contractor. - None

(5) Annex

(a) Total amount of contract is 26 K$. Payment for second quater is $6.500. So the amount of unused funds remaining on the contract at the end of the period covered by the report is $0.

(b) A list of important property acquired with contract funds during this period.

No	List of important properties	Amount, $
1	Salary	3100
2	*Social taxes on salaries and wagess*	1255.5
3	*Expendable Supplies*	1505

ATTACHMENT 5 **Publications**

1. Belov N.N., Belov P.N. Method of probe particles for PC modelling of the aerosol dispersion in turbulence atmosphere for complicated landscape. Sent to 5th International Aerosol Conference, UK, Edinburgh, 12-18 Spt.1998.
2. Belov N.N., Belov P.N. Numerical method for synthetic model of dispersion of aerosols in boundary layer of atmosphere for complicated landscape. Sent to 5th International Aerosol Conference, UK, Edinburgh, 12-18 Spt.1998.
3. Belov N.N., Belov P.N. New method for PC modelling of the aerosol dispersion in turbulence atmosphere on complicated landscape. Sent to 5th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Greece, Rhodes, Greece, 18-21 May 1998.
4. Belov N.N., Belov P.N. PC modelling of the aerosol dispersion in turbulence atmosphere on complicated landscape. Sent to 5th International Aerosol Conference, UK, Edinburgh, 12-18 Spt.1998. Sent to Second International Symposium on Measuring Techniques for Multiphase Flows, China, Beijing, 30.08-1.09.1998.

METHOD OF PROBE PARTICLES FOR PC MODELLING OF THE AEROSOL DISPERSION IN TURBULENCE ATMOSPHERE FOR COMPLICATED LANDSCAPE.

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KEYWORDS

Atmosphere; aerosol dispersion; streamlines; 3D Navier-Stokes equations

PC modelling of the aerosol plume dispersion in atmosphere is very important for ecology. It is very important to find real-time information about transfer of dangerous aerosol plume in atmosphere after incident with chemical or energetical plant. Results of aerosol field experiments closely defined from information about aerosol transfer in atmosphere. Great number of human activities connected with aerosol plumes, with its evolution in turbulence atmosphere. Most important and most difficult for evaluation is zone near aerosol source (1-15 kilometres). Inside this distance aerosol plume closely depends from orography. Inside of this distance aerosol plume has small dispersion. It sizes are compatible with sizes of buildings , mountains,... Direct calculation of this gas dynamical situation is extremely complicated. It is impossible now to obtain good estimation of this task by finite differences method PC calculation. So most important case - the evaluation of the aerosols under complicated surface and near aerosol generator - up to now has not any decision. This investigation devoted to preparing effective methods of investigation of transport of aerosol plume inside of near -zone (1-15 kilometres from source) for complicated orography.

Synthetical model of aerosol transport modelling for the complicated orography.

Most difficult problem of modelling of aerosol transport connected with complicated air streams near buildings, mountains etc. in Boundary layer. The evaluation of aerosol transport may be calculated by several methods with good precision, Smirnov (1996) only after the elevation of the aerosol clouds by convection and large whirlwinds under buildings and another obstacles. Moving the aerosol plume near source depends from different airstreams. So the most important part of this modelling is way of aerosol stream between and near buildings ...

Real time investigation of these complicated air streams is impossible before averawing of the aerosol in this streamlines. It is unknown method for fast and accurate direct solving of 3D aerodynamics problem with complicated boundary conditions.

First step for solving of this problem was made in synthetical modelling of aerosol dispersion in atmosphere, Belov (1998). In this investigation used storage of aerodynamics stream line for great number of elementary air flows for different buildings, group of buildings... 3D computation was used for preparing of the library of the flow lines for great number of obstacles. This library prepared BEFORE modelling of the aerosol plume dispersion provides field of air flows for great number of obstacles. One of these streamlines which moves through place of aerosol generator provides axes line for Gaussian model of aerosol plume dispersion.

Well known Gaussian models for evaluation of the aerosol dispersion in atmosphere are fast and simple. These models may be applied for great numbers of

types of atmosphere conditions. Wind, convection, temperature distribution, sun radiation... - great number of parameters may be used by this model with good results. But all calculations may be fulfilled for plane Earth surface only. This limitation reduces of significance of these models. Most interesting and important aerosol plume problems concern with people, with their houses and industry. These places suited mostly inside of towns. For these places Gaussian models nobody applied before. Our modification of the Gaussian model provides new opportunities for this class of modelling of aerosol dispersion in turbulence atmosphere.

Gaussian models provides quasi - homogeneous aerosol distribution inside of aerosol plume. It is great defect of this model. Most important properties of aerosol plume (optical, chemical...) concerned with great discontinuity of aerosols.

Description of novel aerosol transport modelling for the complicated orography.

Most important results of our investigation concerned with spotted technology of description of the evolution of aerosol flow in turbulence atmosphere. Modelling of the evolution of the aerosol spots is very important for aerosol optics, for modelling of aerosol measurement in real atmosphere. For this purposes it was used method of probe clouds. Each spherical small cloud generated from nozzle of aerosol generation moves by streamlines which was provides from streamlines library. Stochastic generation of these clouds, its transformation by turbulence diffusion, convection and by disturbing by whirlwind near obstacles was used. This method provides good results with standard Pentium PC and CD ROM library.

Conclusion

This investigations provides the possibility of evaluation of more complicated problem of aerosol transport in turbulence atmosphere. Moreover some evaluation of the aerosol dispersion may be made during field experiment in quasi-real time.

ACKNOWLEDGEMENTS

We would like to acknowledge Dr. Birenzvige Amnon for his help with selection of most actual directions of investigations for US Army foundation, for discussion of these results. Many thanks to Mr Jerry C. Comati (44-0171-5144902) chief of environmental science branch of ERO for his supporting of this contract and sponsoring of International Aerosol Symposium in S.Petersburgh (6-9 July 1998).

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We would like to acknowledge the Aerosol Technology Ltd for financial support of airstreams library and PC codes preparation for aerosol dispersion plume by algorithms discussed above. These PC codes and cheap notebook provide great flexibility with investigations of natural aerosol flows for field experiments. *To purchase this new aerosol software please contact Aerosol Technology Ltd (FAX:+7(095)-1474361).*

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Belov N.N., Belov P.N.,Birenzvige A., Synthetical Gaussian plume model of aerosol dispersion by atmosphere, sent to AAAR'98.

Smirnov N.N., Nikitin V.F., Legros J.C., Mathematical modelling of the aerosols evolution and sedimentation in the atmosphere of big cities *J. Aerosol Sci* ., 96 S597-S598.

NUMERICAL METHOD FOR SYNTHETIC MODEL OF DISPERSION OF AEROSOLS IN BOUNDARY LAYER OF ATMOSPHERE FOR COMPLICATED LANDSCAPE.

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KEYWORDS

Final-difference scheme; 3D Navier-Stokes equation; atmosphere; aerosol dispersion

Simulating the dispersion of aerosol in boundary layer of atmospheric is a complex problem that includes analysis of various air flows near the ground and obstacles. Route of aerosol stream strongly depends on landscape and placement of large artificial objects. At most cases Earth shape cannot be described using various coefficients in simple equations for aerosol transport. Most important and most difficult for evaluation is zone around the aerosol source in range of 2-15 kilometers. The synthetic model of aerosol dispersion [Belov(1998)] in atmosphere simulates aerosol transport for any distance if all air flows are known. Meteorological measurements are not acceptable for this model because of too few details of three dimensional air flows are available. Experimental work on measuring all of the flows velocity and structure is hard. To produce such information numerical methods are used.

The present method is based upon the finite-differences scheme for tree dimensional Navier-Stokes gasdynamics equations for homogeneous temperature field. In lower atmosphere absolute values of variations of air pressure (and density) are much less than the average value. This can be used to simplify the Navier-Stokes equations:

$$(1)\ \rho_{av}\cdot\left(\frac{\partial v}{\partial t}+v\frac{\partial v}{\partial x}+u\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=-\frac{p_{av}}{\rho_{av}}\cdot\frac{\partial\rho_{vr}}{\partial x}+\tfrac{4}{3}\eta\cdot\frac{\partial^2 v}{\partial x^2}+\eta\cdot\left(\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)+\tfrac{1}{3}\eta\cdot\left(\frac{\partial^2 u}{\partial x\partial y}+\frac{\partial^2 w}{\partial x\partial z}\right)$$

$$(2)\ \rho_{av}\cdot\left(\frac{\partial u}{\partial t}+v\frac{\partial u}{\partial x}+u\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{p_{av}}{\rho_{av}}\cdot\frac{\partial\rho_{vr}}{\partial y}+\tfrac{4}{3}\eta\cdot\frac{\partial^2 u}{\partial y^2}+\eta\cdot\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial z^2}\right)+\tfrac{1}{3}\eta\cdot\left(\frac{\partial^2 v}{\partial x\partial y}+\frac{\partial^2 w}{\partial y\partial z}\right)$$

$$(3)\ \rho_{av}\cdot\left(\frac{\partial w}{\partial t}+v\frac{\partial w}{\partial x}+u\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=-\frac{p_{av}}{\rho_{av}}\cdot\frac{\partial\rho_{vr}}{\partial z}+\tfrac{4}{3}\eta\cdot\frac{\partial^2 w}{\partial z^2}+\eta\cdot\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}\right)+\tfrac{1}{3}\eta\cdot\left(\frac{\partial^2 v}{\partial x\partial z}+\frac{\partial^2 u}{\partial y\partial z}\right)$$

$$(4)\ \frac{\partial\rho_{vr}}{\partial t}+\rho_{av}\cdot\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}+\frac{\partial w}{\partial z}\right)+v\cdot\frac{\partial\rho_{vr}}{\partial x}+u\cdot\frac{\partial\rho_{vr}}{\partial y}+w\cdot\frac{\partial\rho_{vr}}{\partial z}=0$$

Here V=(v,u,w) is air velocity, p_{av} – average value of pressure, p_{vr} – variation of average value of pressure, $p=p_{av}+p_{vr}$, ρ_{av} – average value of density, ρ_{vr} – average value of density, $\rho=\rho_{av}+\rho_{vr}$, η – dynamic air viscosity.

These partial derivative equations are nonlinear. To solve them, to find air velocity and density, final differences scheme is used. In order to reduce scheme round-off errors, in equations (1)-(3) are divided by density variation ρ_{vr} and introducing the air kinematic viscosity $\nu = \eta / \rho_{vr}$. To copmpute values on each new time step the interation process is initiated. In equations (1)-(3) nonlinear terms treated as production of values from new estimation and the previous one. Estimations are computed by solving matrix 4x4 for linear algebraic equations. The values from previous time step play role of first estimation.

Shorted form for the scheme is:

$$(5)\ v_{\bar{t}} + v\,v_{\bar{x}} + uv_{\bar{y}} + wv_{\bar{z}} = -\frac{p_{av}}{\rho_{av}^2}\cdot(\rho_{vr})_{\bar{x}} + \tfrac{4}{3}\nu\cdot v_{\bar{x}x} + \nu\cdot\left(v_{\bar{y}y} + v_{\bar{z}z}\right) + \tfrac{1}{3}\nu\cdot\left(u_{\bar{x}\bar{y}} + w_{\bar{x}\bar{z}}\right)$$

$$(6)\ u_{\bar{t}} + v\,u_{\bar{x}} + uu_{\bar{y}} + wu_{\bar{z}} = -\frac{p_{av}}{\rho_{av}^2}\cdot(\rho_{vr})_{\bar{y}} + \tfrac{4}{3}\nu\cdot u_{\bar{y}y} + \nu\cdot\left(u_{\bar{x}x} + u_{\bar{z}z}\right) + \tfrac{1}{3}\nu\cdot\left(v_{\bar{x}\bar{y}} + w_{\bar{y}\bar{z}}\right)$$

$$(7)\ w_{\bar{t}} + v\,w_{\bar{x}} + uw_{\bar{y}} + ww_{\bar{z}} = -\frac{p_{av}}{\rho_{av}^2}\cdot(\rho_{vr})_{\bar{z}} + \tfrac{4}{3}\nu\cdot u_{\bar{z}z} + \nu\cdot\left(w_{\bar{x}x} + w_{\bar{y}y}\right) + \tfrac{1}{3}\nu\cdot\left(v_{\bar{x}\bar{z}} + u_{\bar{y}\bar{z}}\right)$$

$$(8)\ (\rho_{vr})_{\bar{t}} + \rho_{av}\cdot(v_{\bar{x}} + u_{\bar{y}} + w_{\bar{z}}) + v\cdot(\rho_{vr})_{\bar{x}} + u\cdot(\rho_{vr})_{\bar{y}} + w\cdot(\rho_{vr})_{\bar{z}} = 0$$

Lower index x mean finite-differential derivative. Ex: $v_{\bar{x}} = \dfrac{V(i,j,k,m) - V(i-1,j,k,m)}{h_{x,i}}$

This method was successfully implemented and tested on problem of horizontal wind which velocity increases with height. Bondary conditions can be of three kinds: 1-given functions (velocity and density), 2-hard surface, 3-free air. Boundary conditions are constructed for each net node separately. Format of description lets add new boundary conditions. Using this technique non-usual conditions may be specified.

ACKNOWLEDGEMENTS

We would like to acknowledge Dr. Birenzvige Amnon for his help with selection of most actual directions of investigations for US Army foundation, for discussion of these results. Many thanks to Mr Jerry C. Comati (fax 44-0171-5144902) chief of environmental science branch of ERO for his supporting of this contract and sponsoring of International Aerosol Symposium in S.Petersburgh (6-9 July 1998).
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Present investigation devoted to the new method for fast and accurate direct solving of 3D aerodynamics problem with complex boundary conditions. The synthetical modelling of aerosol dispersion in atmosphere is based upon the library of streams. Library contains three dimensional description of air flows. The library of flows must be big enough to contain flows around various kinds of obstacles with high precision. Each flow is modelled using final-differences scheme for three dimensional Navier-Stokes equations (without temperature). Final-differences scheme precision could be improved by dividing dynamics equations by value of average density and introducing the kinematic viscosity of air. The last replaces theoretical artificial viscosity so it is not needed. Preparation of library takes a lot of time. But when library is ready computational time needed for synthetic model is small enough to let use of this model during outdoor experimental studies.

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KEYWORDS

Atmosphere; modelling; aerosol dispersion; 3D quasi-real time modelling.

PC modelling of the aerosol plume dispersion in atmosphere is very important. This investigation devoted to preparing effective methods of prediction of aerosol transport in area around the aerosol source (1-15 kilometres) for complicated orography. Known models of aerosol transport can not be realised for complicated air streams near buildings, excavations, mountains and other parts of landscape has significant influence on trajectory of air streams. On small distances averaging of land surface leads to serious loose of precision. Aerosol transport may be evaluated by several methods with good precision only after the elevation of the aerosol clouds and their transported over the obstacles. Local convection flows and whirlwinds near obstacles modifies concentration field. This variation is too small if the source of aerosol is far from the investigated area. But concentration near the source can be very high at one place and there can be no aerosol at the another. Movement of the aerosol plume near source depends from different air streams. So the most important part of modelling is description of aerosol streams and thier route from the source.

Present investigation devoted to the new method for fast and accurate direct solving of 3D aerodynamics problem with complex boundary conditions. The synthetical modelling described in Belov et all (1998) of aerosol dispersion in atmosphere is based upon the storage of descriptions of aerodynamics streamlines for great number of elementary air flows for parts of landscape, buildings and their groups. The library of streams contains three dimensional description of air flows for great number of obstacles. Each flow was modelled using final-differences scheme for three dimensional Navier-Stokes equations (without temperature) which is described in Belov et all (1998). Preparation of this library takes a lot of time. But when library is ready computational time needed for synthetic model is small enough to let use of this model during outdoor experimental studies.

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ACKNOWLEDGEMENTS

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